

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
 Data File : BF126591.D
 Acq On : 11 Jan 2022 14:45
 Operator : JU/CG
 Sample : N1054-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220016-CAPE-3-COMP

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126591.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.363	383	387	394	rBV	44170	57923	1.88%	0.280%
2	5.016	494	498	507	rVB	41520	60830	1.97%	0.294%
3	5.398	557	563	566	rBV	2593822	2898120	93.84%	14.004%
4	6.410	729	735	738	rBV	2396485	3088274	100.00%	14.923%
5	6.769	792	796	799	rBV	630685	540585	17.50%	2.612%
6	7.333	886	892	895	rBV	1800831	1992312	64.51%	9.627%
7	7.957	993	998	1009	rBV	287419	282684	9.15%	1.366%
8	8.051	1009	1014	1017	rVV	820787	781502	25.31%	3.776%
9	9.133	1191	1198	1201	rBV	2668195	3032070	98.18%	14.651%
10	9.810	1307	1313	1316	rBV	849809	848440	27.47%	4.100%
11	10.604	1440	1448	1451	rBV	1888766	2013269	65.19%	9.728%
12	11.292	1561	1565	1569	rBV	899795	818118	26.49%	3.953%
13	11.833	1653	1657	1667	rBV2	76918	88650	2.87%	0.428%
14	12.892	1831	1837	1840	rBV	2557562	2598081	84.13%	12.554%
15	13.792	1986	1990	2002	rBV3	145545	256507	8.31%	1.239%
16	13.939	2011	2015	2019	rVB	704496	667931	21.63%	3.228%
17	14.039	2025	2032	2038	rBV	53821	57547	1.86%	0.278%
18	15.404	2259	2264	2269	rBV	460211	576352	18.66%	2.785%
19	15.868	2338	2343	2349	rBV	23525	35748	1.16%	0.173%

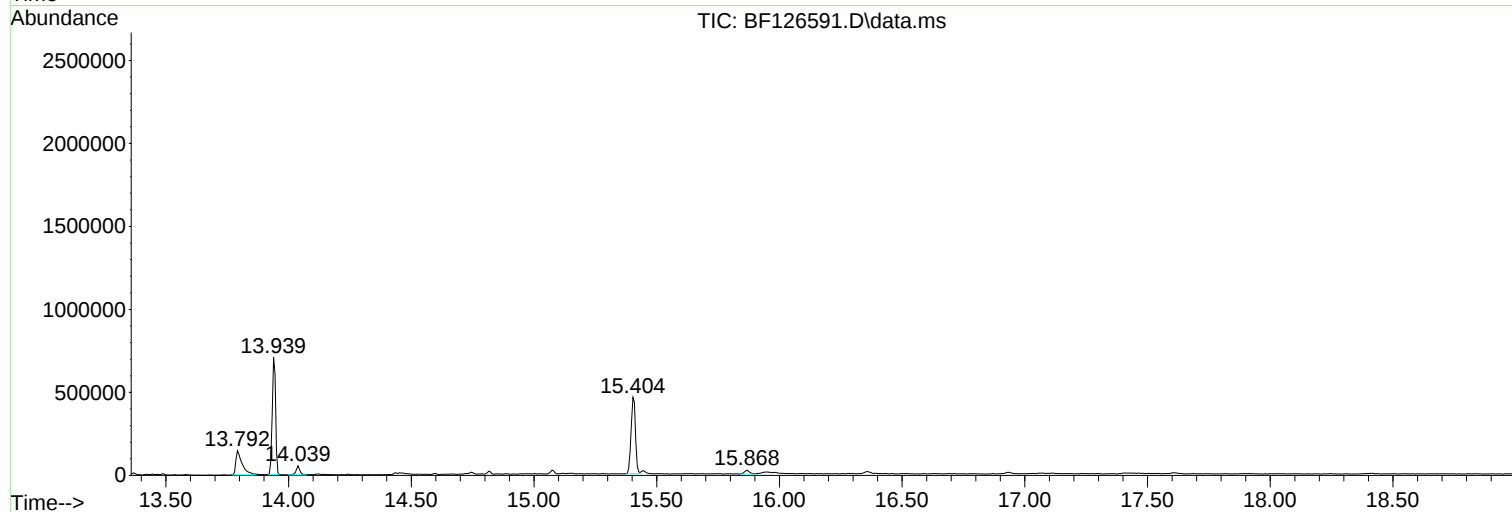
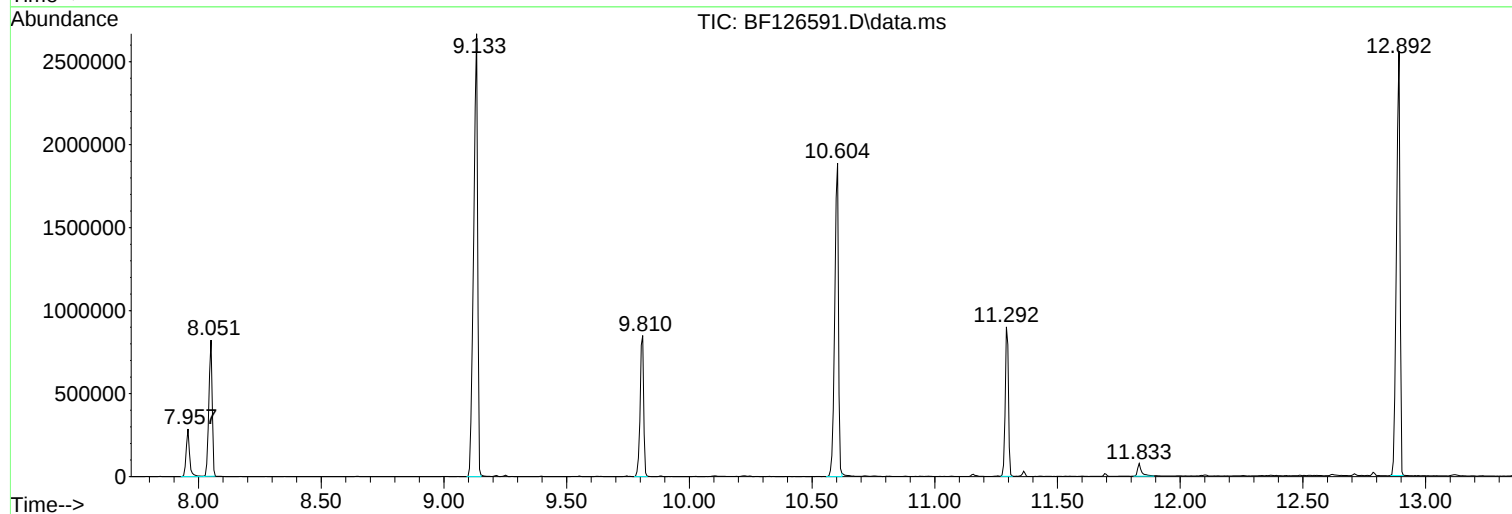
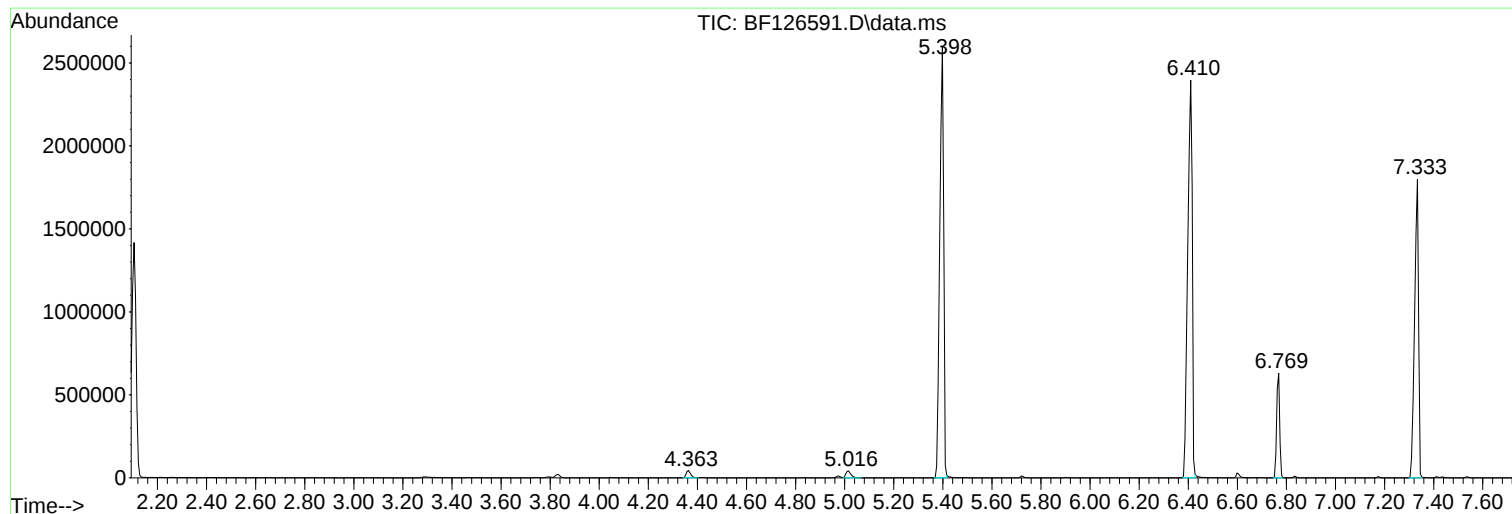
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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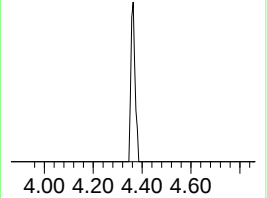
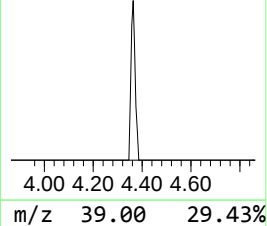
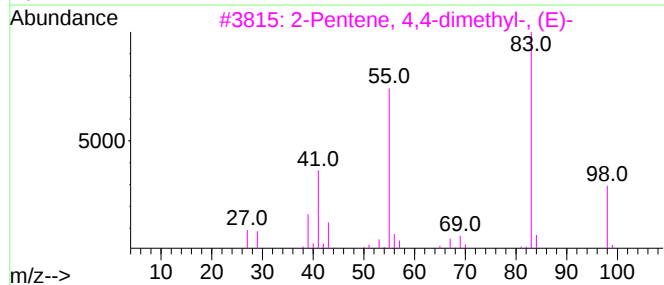
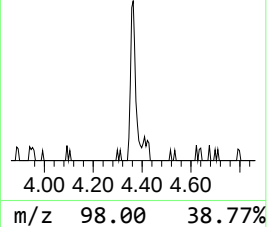
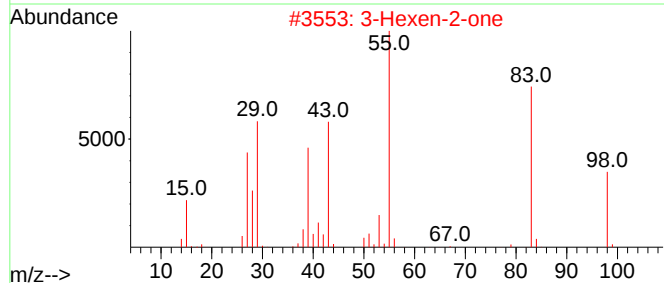
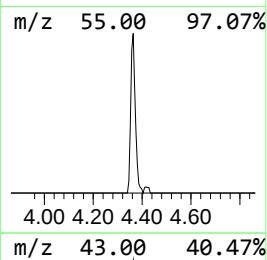
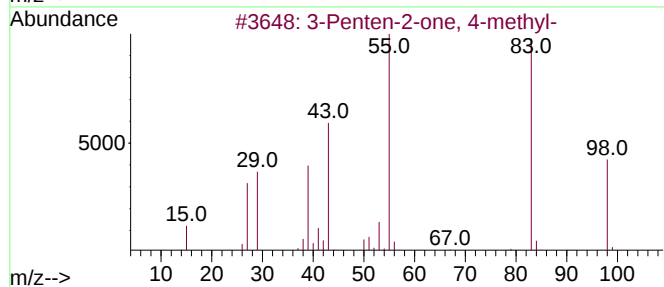
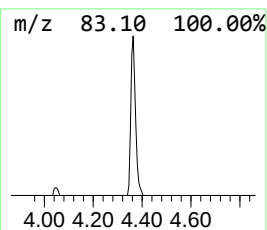
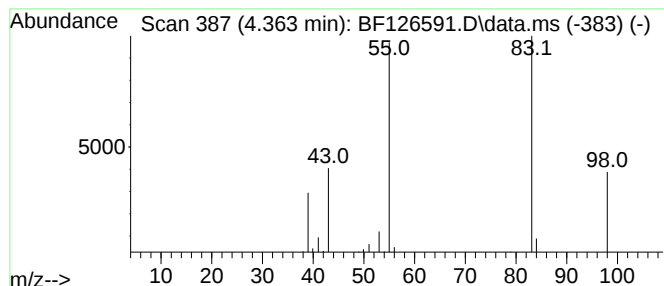
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.363	2.14 ng	57923	1,4-Dichlorobenzene-d4	6.769

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72



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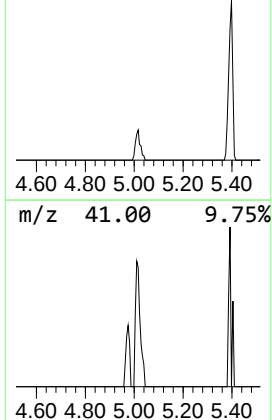
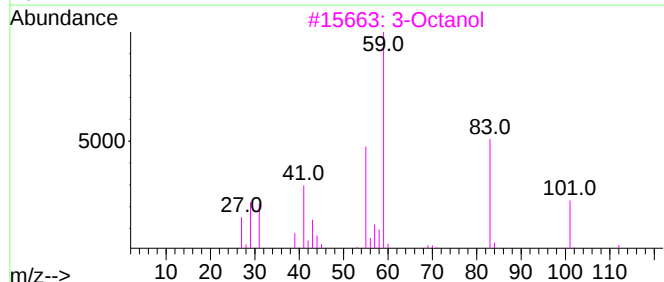
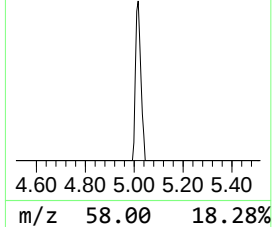
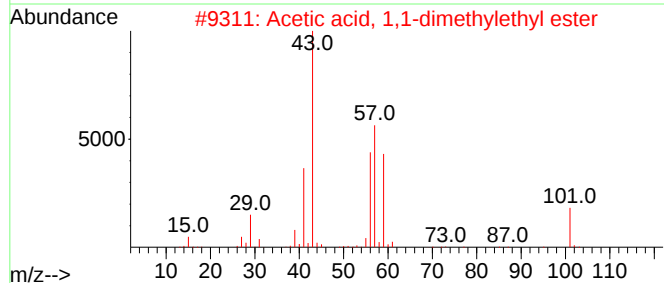
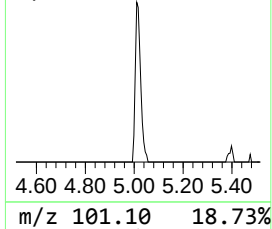
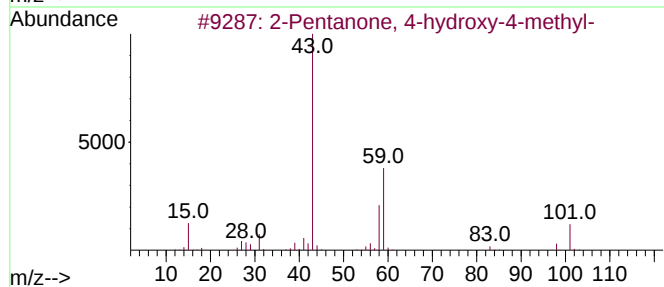
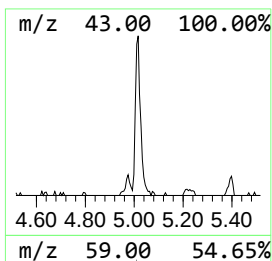
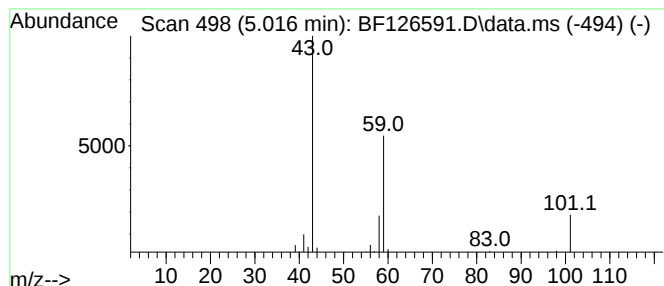
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	2.25 ng	60830	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Octanol	130	C8H18O	000589-98-0	36
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23



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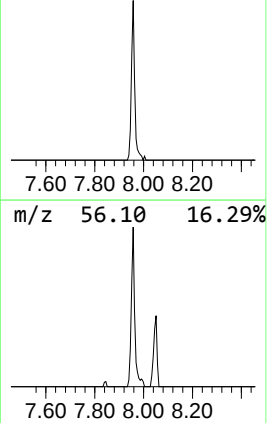
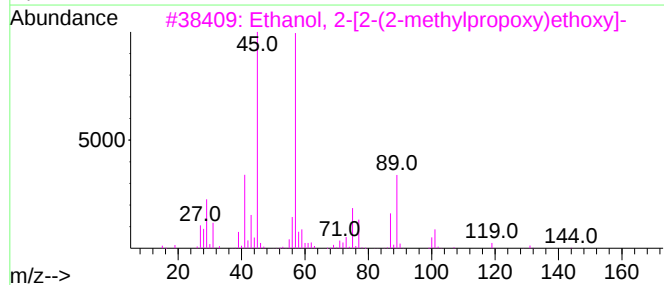
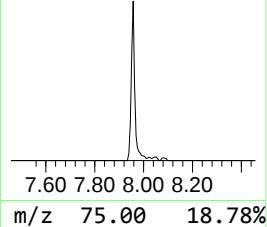
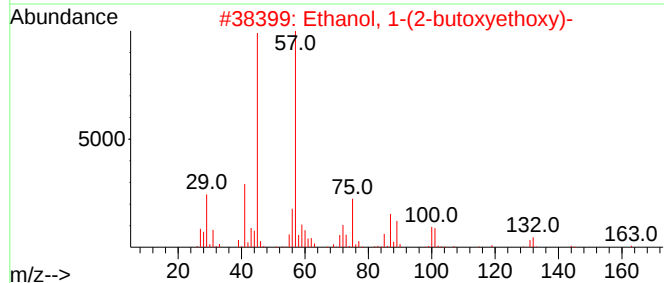
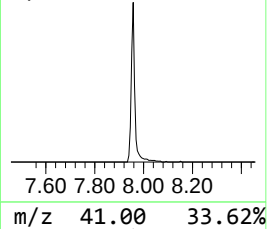
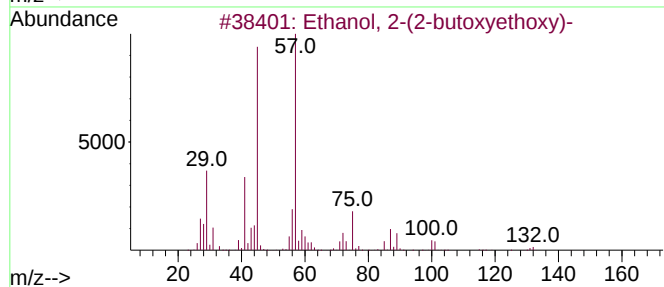
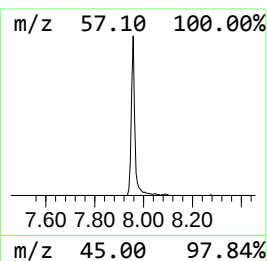
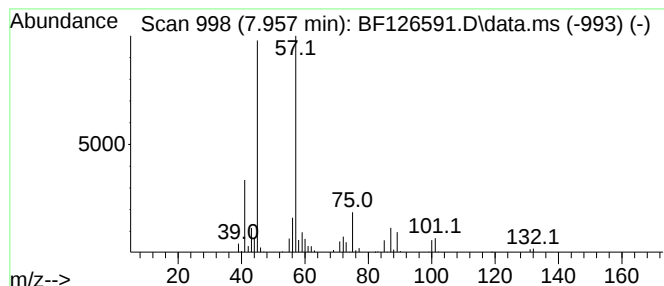
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.957	7.23 ng	282684	Naphthalene-d8	8.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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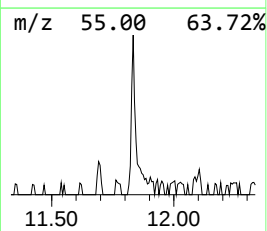
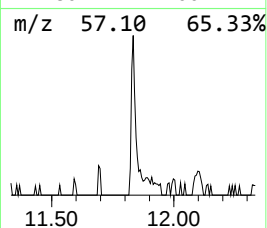
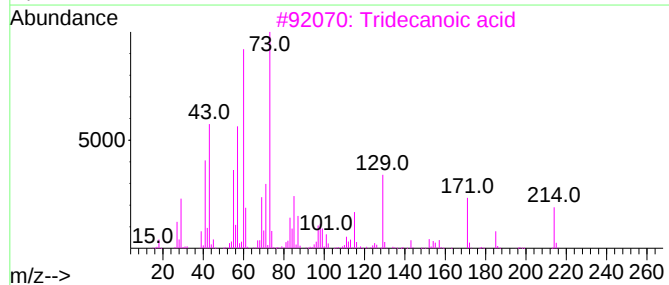
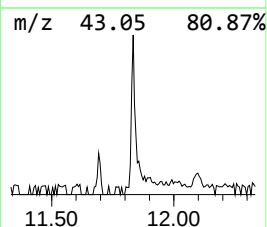
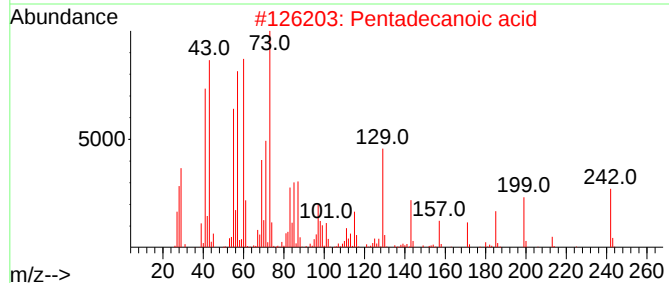
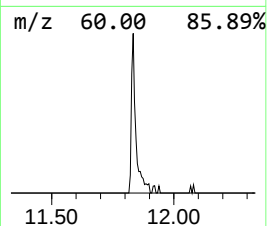
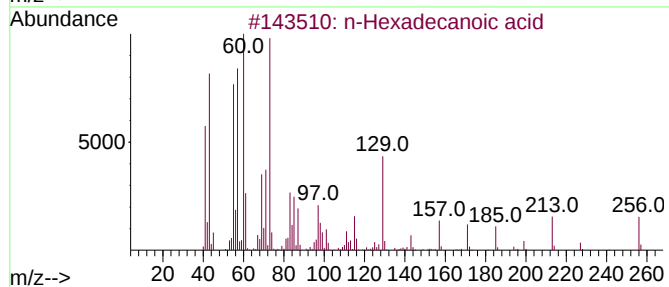
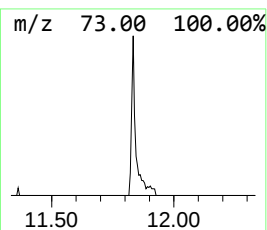
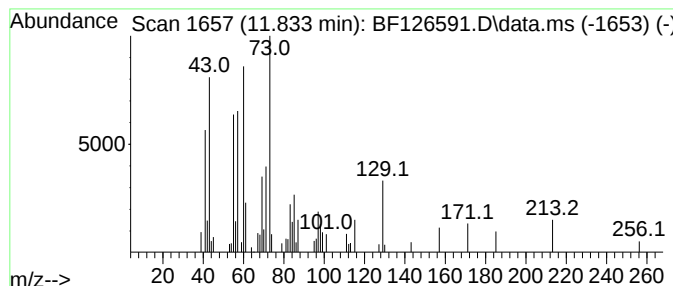
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	2.17 ng	88650	Phenanthrene-d10	11.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	18
5			Pentadecane	212	C15H32	000629-62-9	11



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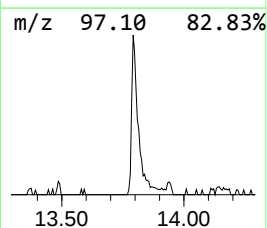
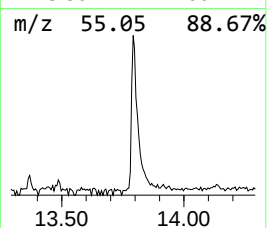
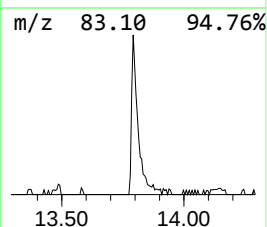
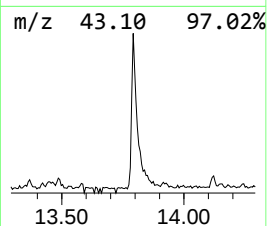
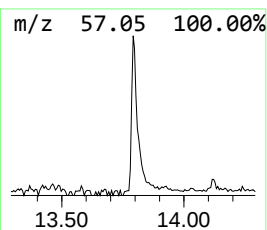
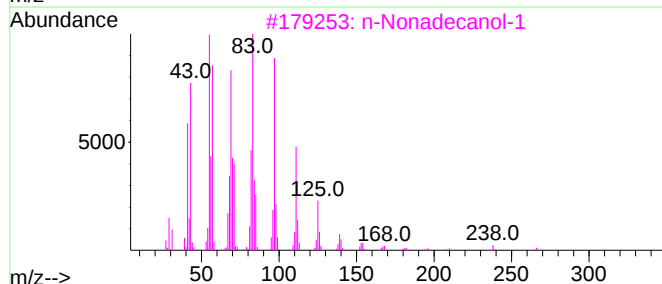
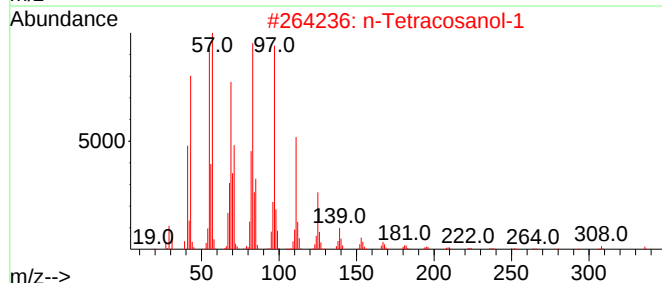
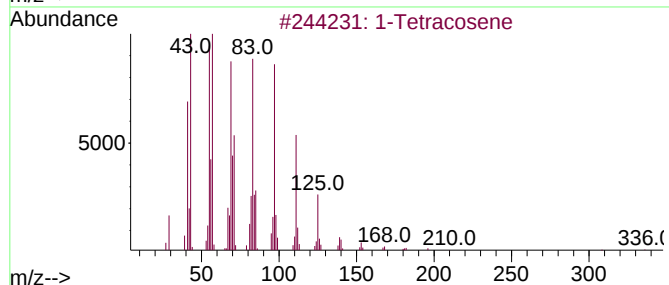
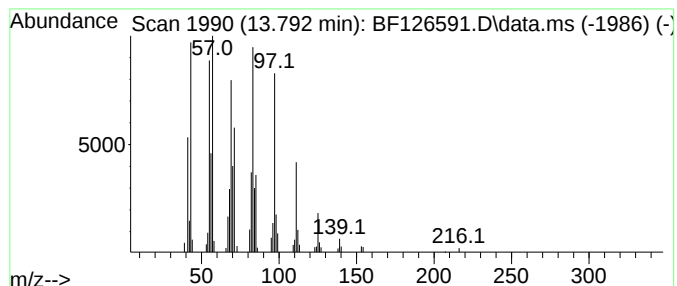
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Tetracosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.792	7.68 ng	256507	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	91
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4			1-Heneicosanol	312	C21H44O	015594-90-8	91
5			1-Heptacosanol	396	C27H56O	002004-39-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.363	2.1	ng	57923	1	6.769	540585	20.0
2-Pentanone, 4-...	5.016	2.3	ng	60830	1	6.769	540585	20.0
Ethanol, 2-(2-b...	7.957	7.2	ng	282684	2	8.051	781502	20.0
n-Hexadecanoic ...	11.833	2.2	ng	88650	4	11.292	818118	20.0
1-Tetracosene	13.792	7.7	ng	256507	5	13.939	667931	20.0